

Simple Analytical Expressions of the Non-Linear Reaction Diffusion Process in an Immobilized Biocatalyst Particle using the New Homotopy Perturbation Method

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Abstract

In this research article, we demonstrate the application of the New Homotopy perturbation method to work out the nonlinear singular boundary value problems which often arise in chemical and biochemical engineering and scientific disciplines. For demonstration, the reaction-diffusion process occurring in a spherical porous immobilized biocatalyst has been solved successfully with the Michaelis-Menten form of kinetics. Simple analytical expressions of the concentrations and the effectiveness factors are derived by using the New Homotopy perturbation method. Our analytical results are compared with the numerical results and a satisfactory agreement is noted.

Keywords

Biocatalyst; Reaction-diffusion Process; Effectiveness Factor; Thiele Modulus; New Homotopy Perturbation Method; Numerical Simulation

Introduction

The rising interest in the application of biocatalysts entrapped in inert porous supports is mainly ascribable to their high volumetric productivities and the characteristics of being used repeatedly. The effectiveness factor of these immobilized biocatalyst particles is of capital importance in optimizing the processes because usually the diffusion of the substrates into the livelihoods and the products out of the supports have been affected significantly. Many works have been carried out to create mathematical models using the reaction-diffusion equations, which are commonly solved by numerical means (of iterative nature) as there are limited analytical solutions [Li et. al.(2004) and Villadsen et. al (1978)]. On that point are also iterative approximate solutions available in literature, which are obtained by comparison theorems

[Parshotam et. al (1991)]. Another method based on a Taylor series linearization technique was given for a biofilm reactor with Monod kinetics and product inhibition [Bhaskar et. al (1991), Walas et. al (1995) and Silva et. al (2001)].

In this paper, a simple analytical expression is suggested to identify the substrate concentration distribution inside the immobilized biocatalyst particles and further to estimate their effectiveness factor. This offers an option for fast estimation of such a parameter in practice.

Mathematical Formulation Of The Boundary Value Problem

The immobilized spherical biocatalyst particle of the mass transfer is ordered by the Fick's first law and the biochemical reaction follows the Michaelis -Menten kinetics, the reaction-diffusion process of substrate in the particle at steady state may be written every bit:

$$\frac{d^2C}{dr^2} + \frac{2}{r} \frac{dC}{dr} - \frac{r_m C}{D(K_m + C)} = 0 \quad (1)$$

To reduce the eqn.(1) into the normalized form, we use the following dimensionless variables:

$$y = \frac{C}{C_s}, \quad x = \frac{r}{R}, \quad \beta = \frac{C_s}{K_m}, \quad \varphi = \frac{R}{3} \sqrt{\frac{r_m}{DK_m}} \quad (2)$$

Now, the eqn. (1) become

$$\frac{d^2y}{dx^2} + \frac{2}{x} \frac{dy}{dx} - 9\varphi^2 \left(\frac{y}{1 + \beta y} \right) = 0 \quad (3)$$

The corresponding boundary conditions of the eqn. (3) are

$$\frac{dy}{dx} = 0 \text{ at } x = 0 \quad (4)$$

$$y = 1 \text{ at } x = 1 \quad (5)$$

The second boundary condition assumes the external convection resistance is neglected. By the definition of the effectiveness factor for a spherical immobilized biocatalyst, an equation of it is

$$\eta = \frac{4\pi R^2 D (dC/dr)_{r=R}}{(4/3)\pi R^3 (r_m C_s / (K_m + C_s))} \quad (6)$$

$$\eta = \frac{\beta + 1}{3\phi^2} \left(\frac{dy}{dx} \right)_{x=1} \quad (7)$$

Analytical Expression Of The Normalized Surface Concentrations Using The New Homotopy Perturbation Method

Linear and non-linear phenomena are of fundamental importance in various fields of science and engineering. Most models of real life problems are still very difficult to solve. Therefore, approximate analytical solutions such as a Homotopy perturbation method (HPM) [Gohri et. al (2007), Ozis et. al (2007), Li et. al (2006), Mousa et. al (2008), He (1999 and 2003), Ariel (2010), Ananthaswamy et. al (2012 and 2013) and Shanthi et. al (2013)] were introduced. This method is the most effective and convenient one for both linear and non-linear equations. Perturbation method is based on assuming a small parameter. The majority of non-linear problems, especially those having strong non-linearity, have no small parameters at all and the approximate solutions obtained by the perturbation methods, in most cases, are valid only for small values of the small parameter. Generally, the perturbation solutions are uniformly valid as long as a scientific system parameter is small. However, we cannot rely fully on the approximations, because there is no criterion on which the small parameter should exist. Thus, it is essential to check the validity of the approximations numerically and/or experimentally. To overcome these difficulties, HPM have been proposed recently.

Recently, many authors have applied the Homotopy perturbation method (HPM) to solve the nonlinear boundary value problem in physics and engineering sciences [Gohri et. al (2007), Ozis et. al (2007), Li et. al (2006), Mousa et. al (2008)]. Recently this method is also used to solve some of the non-linear problem in physical sciences [Mousa et. al (2008), He (1999 and 2003)]. This method is a combination of Homotopy in

topology and classic perturbation techniques. Ji-Huan He used to solve the Lighthill equation [Mousa et. al (2008)], the Diffusion equation [He (1999)] and the Blasius equation [He (2003)]. The HPM is unique in its applicability, accuracy and efficiency. The HPM and New HPM [Gohri et. al (2007), Ozis et. al (2007), Li et. al (2006), Mousa et. al (2008), He (1999 and 2003), Ariel (2010), Ananthaswamy et. al (2012 and 2013) and Shanthi et. al (2013)] uses the imbedding parameter η as a small parameter, and only a few iterations are needed to search for an asymptotic solution. The approximate analytical expression of concentration (see Appendix B) of the icons. (3)-(5) using the New Homotopy perturbation method [Ananthaswamy et. al (2012 and 2013), Shanthi et. al (2013)] is given by

$$y = \frac{\sinh(kx)}{x \sinh(k)} \quad (8)$$

The corresponding effectiveness factor η can be calculated by using the eqn. (7) is as follows:

$$\eta = \left(\frac{(\beta + 1)}{3\phi^2 \sinh(k)} \right) (k \cosh(k) + \sinh(k)) \quad (9)$$

where k is defined by

$$k = \frac{3\phi}{\sqrt{1 + \beta}} \quad (10)$$

Numerical Simulation

The non-linear reaction-diffusion equations (3)-(5) are also solved by numerically. We have used the function `pdex4` in Scilab/Matlab numerical software to solve numerically, the initial-boundary value problems for parabolic-elliptic partial differential equations. This numerical solution is compared with our analytical results (Figs. (1)-(2)).

Results And Discussions

Figure.1 shows the dimensionless substrate concentration $y(x)$ versus the dimensionless radial distance x . From these Figs. it is clear that when the dimensionless Michaeliss-Menten constant β increases, the corresponding substrate concentration $y(x)$ also increases for various values of the Thiele modulus ϕ^2 . Figure.2 also shows the dimensionless substrate concentration $y(x)$ versus the dimensionless radial distance x . From these Figs. we infer that when the Thiele modulus ϕ^2 increases, the corresponding dimensionless substrate concentration $y(x)$ decreases for various values of the dimensionless Michaeliss-

Menten constant β .

Figure. 3 shows the dimensionless effectiveness factors η versus the dimensionless Michaelis-Menten constant β . From these Figs. it is observed that when the Thiele modulus ϕ^2 increases, the corresponding effectiveness factors η also increases. Figure. 4, shows the dimensionless effectiveness factors η versus the

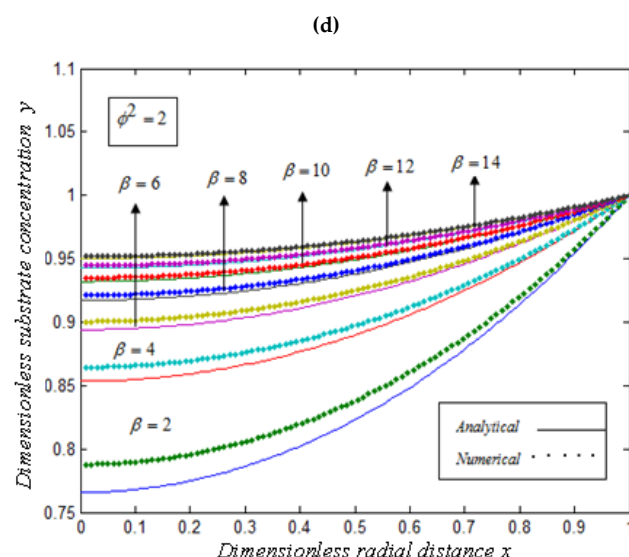
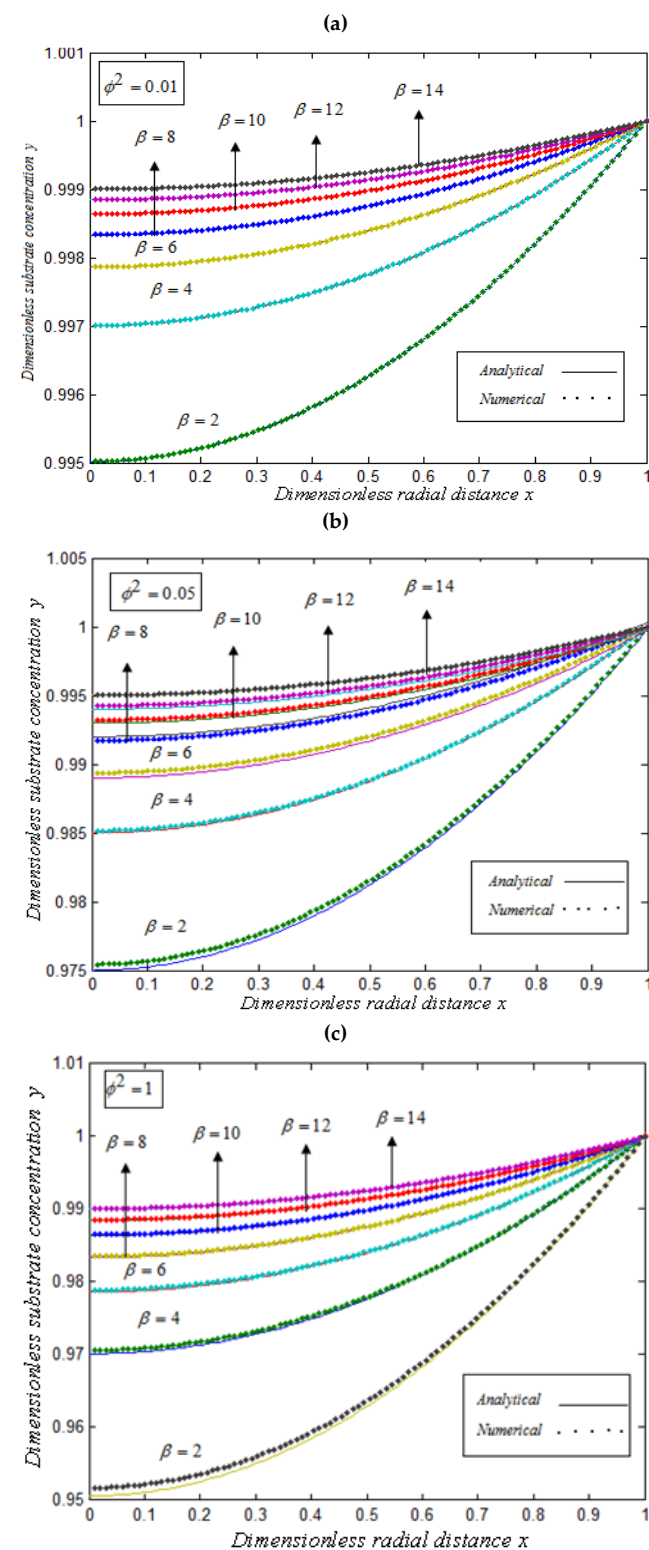
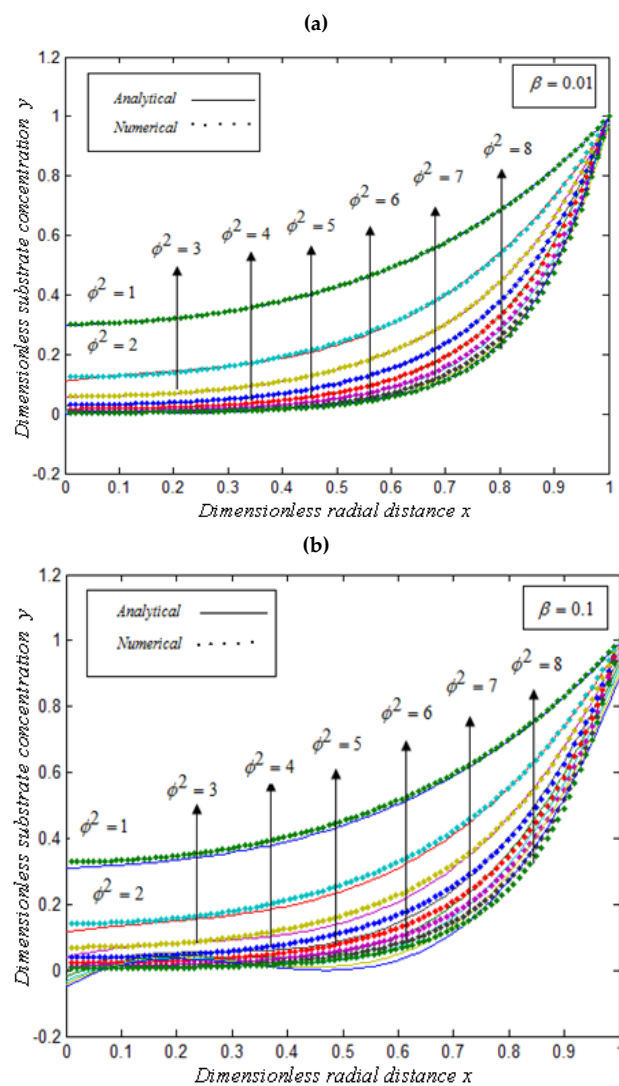


FIGURE 1 DIMENSIONLESS SUBSTRATE CONCENTRATION y VERSUS DIMENSION RADIAL DISTANCE x COMPUTED BY USING THE EQNS. (8) AND (10) FOR ALL VALUES OF THE DIMENSIONLESS MICHAELIS-MENTEN CONSTANT β , AND FOR VARIOUS VALUES OF THE THIELE MODULUS ϕ^2 , WHEN (A) $\phi^2 = 0.01$, (B) $\phi^2 = 0.05$, (C) $\phi^2 = 1$ AND (D) $\phi^2 = 2$.



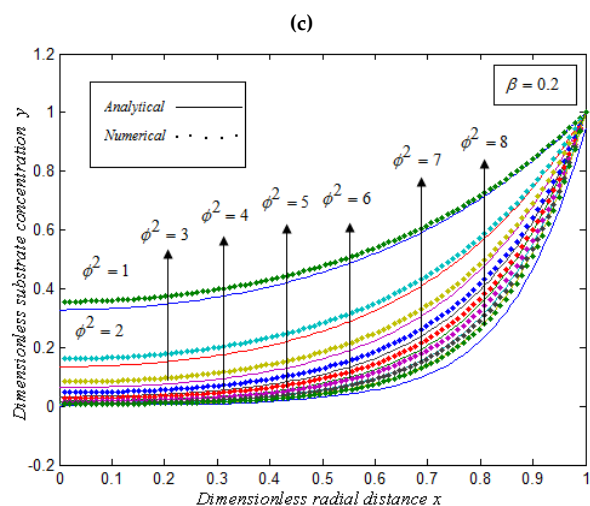


FIGURE 2 DIMENSIONLESS SUBSTRATE CONCENTRATION y VARIOUS DIMENSION RADIAL DISTANCE x COMPUTED BY USING THE EQNS. (8) AND (10) FOR ALL VALUES OF THE OF THE THIELE MODULUS ϕ^2 , AND FOR VARIOUS VALUES DIMENSIONLESS MICHAELISS-MENTEN CONSTANT β , WHEN (A) $\beta = 0.01$, (B) $\beta = 0.1$ AND (C) $\beta = 0.2$.

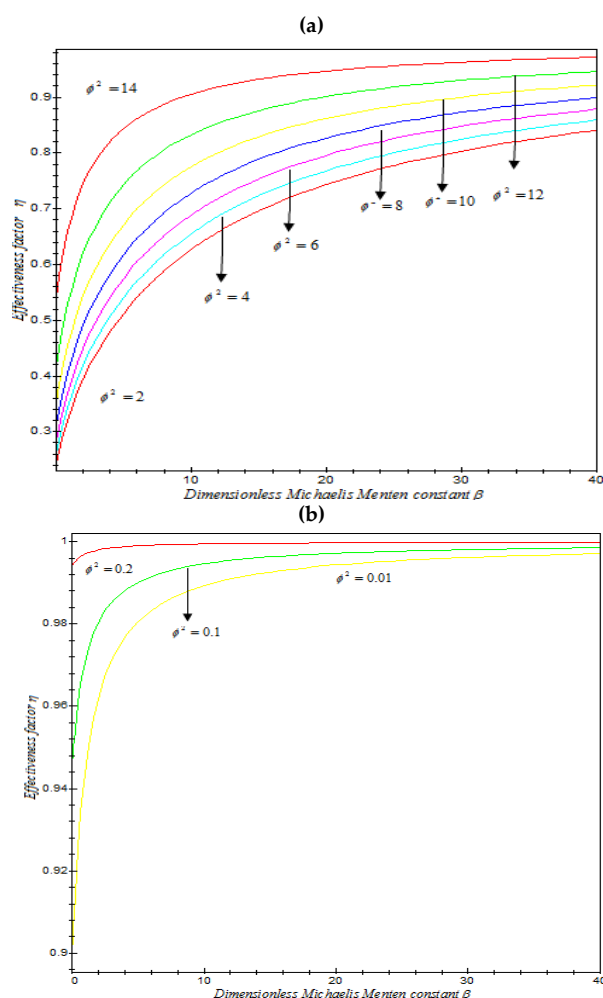


FIGURE 3 DIMENSIONLESS MICHAELISS-MENTEN CONSTANT β VERSUS THE EFFECTIVENESS FACTOR η FOR VARIOUS VALUES OF THE THIELE MODULUS ϕ^2 , WHEN (A) $\phi^2 = 2, 4, 6, 8, 10, 12$ and 14 (B) $\phi^2 = 0.01, 0.1$ and 0.2.

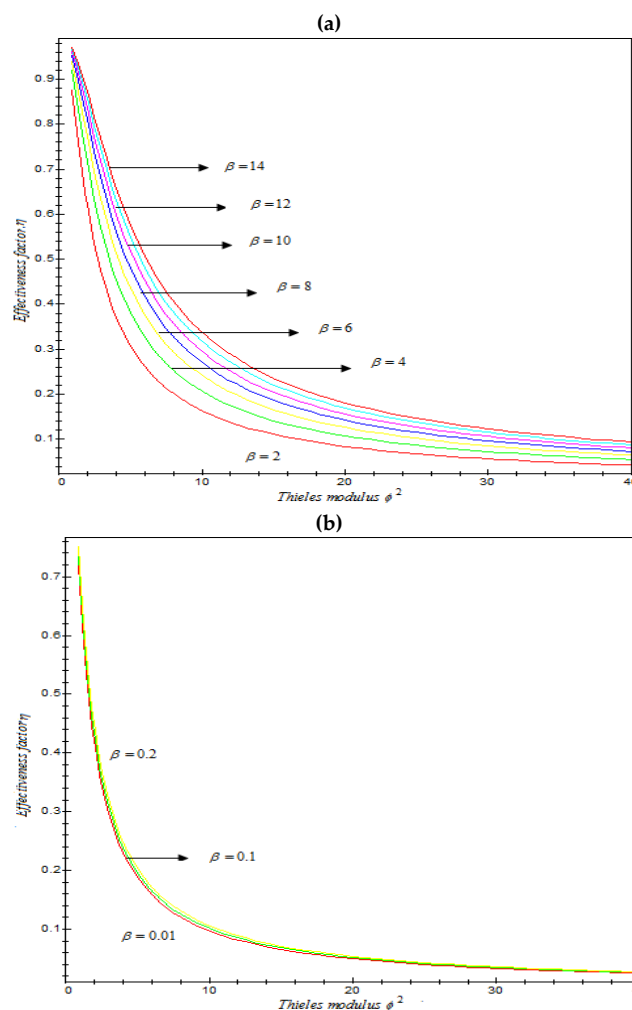


FIGURE 4 THIELE MODULUS ϕ^2 VERSUS THE EFFECTIVENESS FACTOR η FOR VARIOUS VALUES OF THE MICHAELISS-MENTEN CONSTANT β , WHEN (A) $\beta = 2, 4, 6, 8, 10, 12$ and 14, (B) $\beta = 0.01, 0.1$ and 0.2.

dimensionless the Thiele modulus ϕ^2 . From these Figs. we note that when the dimensionless Michaeliss-Menten constant β increases, the corresponding effectiveness factors η also increases.

Conclusions

This research article reports a mathematical treatment for immobilized spherical biocatalyst of the mass transfer. The novelty of this manuscript is an application of approximate method of the second order non-linear partial differential equations. The approximate analytical expressions for the steady state substrate concentration profiles for all values of the dimensionless parameters β and ϕ^2 are obtained using the New Homotopy perturbation method. Furthermore, an analytical expression corresponding to the steady state effectiveness factor is also presented. The effectiveness factors of the biocatalyst

particles may be estimated using the HPM for some values of φ^2 such as oxygen transport into natural mycelia pellets in submerged cultures. A satisfactory agreement with the numerical results is noted. This analytical expression presented in this manuscript can be easily extended too many non-linear reaction-diffusion equations in biosensors.

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Appendix A: Basic Concept Of The Homotopy Perturbation Method

To explain this method, let us consider the following function:

$$D_o(u) - f(r) = 0, \quad r \in \Omega \quad (\text{A.1})$$

with the boundary conditions of

$$B_o(u, \frac{\partial u}{\partial n}) = 0, \quad r \in \Gamma \quad (\text{A.2})$$

where D_o is a general differential operator, B_o is a boundary operator, $f(r)$ is a known analytical function and Γ is the boundary of the domain Ω . In general, the operator D_o can be divided into a linear part L and a non-linear part N . The eqn.(A.1) can therefore be written as

$$L(u) + N(u) - f(r) = 0 \quad (\text{A.3})$$

By the Homotopy technique, we construct a Homotopy $v(r, p): \Omega \times [0, 1] \rightarrow \mathbb{R}$ that satisfies

$$H(v, p) = (1-p)[L(v) - L(u_0)] + p[D_o(v) - f(r)] = 0 \quad (\text{A.4})$$

$$H(v, p) = L(v) - L(u_0) + pL(u_0) + p[N(v) - f(r)] = 0 \quad (\text{A.5})$$

where $p \in [0, 1]$ is an embedding parameter, and u_0 is an initial approximation of the eqn.(A.1) that satisfies the boundary conditions. From the eqns. (A.4) and (A.5), we have

$$H(v, 0) = L(v) - L(u_0) = 0 \quad (\text{A.6})$$

$$H(v, 1) = D_o(v) - f(r) = 0 \quad (\text{A.7})$$

When $p=0$, the eqns.(A.4) and (A.5) become linear equations. When $p=1$, they become non-linear equations. The process of changing p from zero to unity is that of $L(v) - L(u_0) = 0$ to $D_o(v) - f(r) = 0$. We

first use the embedding parameter p as a small parameter and assume that the solutions of the eqns. (A.4) and (A.5) can be written as a power series in p :

$$v = v_0 + pv_1 + p^2v_2 + \dots \quad (\text{A.8})$$

Setting $p=1$ results in the approximate solution of the eqn. (A.1):

$$u = \lim_{p \rightarrow 1} v = v_0 + v_1 + v_2 + \dots \quad (\text{A.9})$$

This is the basic idea of the HPM.

Appendix B: Analytical Solution The Eqns. (3)-(5) Using The New Homotopy Perturbation Method

In this Appendix, we indicate how the eqn. (8) in this paper is derived. To find the solution of eqns.(3) - (5) we construct the new Homotopy as follows [shanthi et. al (2013)]

$$(1-p) \left[\frac{d^2 y}{dx^2} + \frac{2}{\rho} \left(\frac{dy}{dx} \right) - \left(\frac{9\varphi^2}{1+\beta} \right) y \right] + p \left[\frac{d^2 y}{dx^2} + \frac{2}{\rho} \left(\frac{dy}{dx} \right) - \left(\frac{9\varphi^2 y}{1+\beta y} \right) \right] = 0 \quad (\text{B.1})$$

The analytical solution of the eqn.(B.1) is

$$y = y_0 + py_1 + p^2 y_2 + \dots \quad (\text{B.2})$$

Substituting the eqn.(B.2) into an eqn. (B.1) we get

$$(1-p) \left[\frac{d^2 (y_0 + py_1 + p^2 y_2 + \dots)}{dx^2} + \frac{2}{x} \left(\frac{d(y_0 + py_1 + p^2 y_2 + \dots)}{dx} \right) - \left(\frac{9\varphi^2}{1+\beta} \right) (y_0 + py_1 + p^2 y_2 + \dots) \right] + p \left[\frac{d^2 (y_0 + py_1 + p^2 y_2 + \dots)}{dx^2} + \frac{2}{x} \left(\frac{d(y_0 + py_1 + p^2 y_2 + \dots)}{dx} \right) - \left(\frac{9\varphi^2 (y_0 + py_1 + p^2 y_2 + \dots)}{1+\beta(y_0 + py_1 + p^2 y_2 + \dots)} \right) \right] = 0 \quad (\text{B.3})$$

Comparing the coefficients of like powers of p an eqn.(B.3) we get

$$p^0 : \frac{d^2 y_0}{dx^2} + \frac{2}{\rho} \left(\frac{dy_0}{dx} \right) - \left(\frac{9\varphi^2}{1+\beta} \right) y_0 = 0 \quad (\text{B.4})$$

The initial approximations are as follows:

$$y_0'(0) = 0 \text{ and } y_0(1) = 1 \quad (\text{B.5})$$

$$y_i'(0) = 0 \text{ and } y_i(1) = \text{for } i = 1, 2, 3, \dots \quad (\text{B.6})$$

Solving the eqn. (B.4) and using the boundary conditions the eqns.(B.5)-(B.6), we obtain the following results:

$$y = \frac{\sinh(kx)}{x \sinh(k)} \quad (\text{B.8})$$

where k is defined by the text eqn. (10)

According to the HPM, we can conclude that

$$y = \lim_{p \rightarrow 1} y(x) = y_0 \quad (\text{B.9})$$

After putting the eqn.(B.8) into an eqn.(B.9), we obtain the solution in the text eqn.(8).

Appendix C: Matlab/Scilab Program To Find The Solution For The Non-Linear Eqns. (3)-(5)

```
function
m = 2;
x = linspace(0,1);
t = linspace(0,100000);
sol = pdepe(m,@pdex4pde,@pdex4ic,@pdex4bc,x,t);
u1 = sol(:,1);
figure
plot(x,u1(end,:))
title('u1(x,t)')
xlabel('Distance x')
ylabel('u1(x,1)')
function [c,f,s] = pdex4pde(x,t,u,DuDx)
c = 1;
f = 1.* DuDx;
phi=sqrt(0.05);beta=14;
F = -9*(phi)^2*u(1)/(1+(beta*u(1)));
s = F;
function u0 = pdex4ic(x);
u0 = 0;
function [pl,ql,pr,qr] = pdex4bc(xl,ul,xr,ur,t)
pl = 0;
ql = 1;
pr = ur(1)-1;
qr = 0;
```

Appendix D: Nomenclature

Symbol	Meaning
y	Dimensionless substrate concentration
β	Dimensionless Michaelis Menten constant
η	Effectiveness factor
x	Dimensionless radial distance
ϕ	Thiele modulus
C	Substrate concentration
c_s	Substrate concentration on the surface of the particle
D	Effective diffusivity
K_m	Michaelis-Menten constant
r	Radial distance
r_m	Maximum reaction rate`
R	Particle radius

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